

Making Earth Science Data Records for Use in Research Environments (MEaSUREs)

README Document for OMPS_NPP_NMSO2_PCA_L2 OMPS NPP Nadir Mapper SO₂ Level 2 Product Based on PCA Algorithm

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Revision History

09/13/2019, NMSO₂-PCA-L2 product updated from version 1.1 to version 1.2, introducing a new volcanic SO₂ flagging scheme.

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1. INTRODUCTION

1.1 OMPS_NPP_NMSO2_PCA_L2 Product

This document describes the OMPS_NPP_NMSO2_PCA_L2 data product (henceforth shortened to NMSO2-PCA-L2). NMSO2-PCA-L2 is a Level 2, orbital-track volcanic and anthropogenic sulfur dioxide (SO₂) product for the Ozone Mapping and Profiler Suite (OMPS) Nadir Mapper (NM) onboard the NASA/NOAA Suomi National Polar-orbiting Partnership (SNPP) satellite, which was launched on October 28, 2011 into a polar sun-synchronous orbit and has been collecting data since January 2012. As part of the NASA's Making Earth System Data Records for Use in Research Environments (MEaSUREs) program, the Goddard Earth Science (GES) Data and Information Data Center (DISC) has released a new SO₂ Earth System Data Record (ESDR), NMSO2-PCA-L2, processed using the Goddard Space Flight Center (GSFC) Principal Component Analysis (PCA) trace gas retrieval algorithm. NMSO2-PCA-L2 is a Level 2 orbital swath product that spans the entire SNPP/OMPS record. It offers great consistency with the NASA standard Aura/OMI (Ozone Monitoring Instrument, launched in 2004) SO₂ product produced with the same PCA algorithm, and provides continuity between OMI and the follow-up OMPS instrument aboard the NASA/NOAA JPSS-1 satellite (scheduled for launch in November 2017).

1.2 OMPS/SNPP Nadir Mapper

The Nadir Mapper (NM) of OMPS is a nadir-viewing UV spectrometer that measures backscattered solar UV radiance spectra from Earth and solar irradiance in the 300–380 nm wavelength range at a spectral resolution of ~1 nm (Flynn et al., 2014; Seftor et al., 2014). The first model has been flying onboard the NASA/NOAA SNPP spacecraft since 2011, in a sun-synchronous orbit with a

local afternoon equator crossing time of roughly 1:30 p.m. OMPS-NM has a 110° field of view (FOV) and covers a cross-track swath of approximately 2800 km, providing global coverage on a daily basis (14-15 orbits per day). The nominal spatial resolution of OMPS-NM is $50 \text{ km} \times 50 \text{ km}$ at nadir in the nominal observation mode. For about one day every week, the instrument takes measurements in the high spatial resolution mode but at fewer wavelengths. Currently, NMSO₂-PCA-L2 data are limited to the nominal observation mode.

1.3 Science Background

SO₂ is an important air pollutant that has significant impacts on both air quality and climate. It is emitted from both anthropogenic sources (e.g., power plants) and volcanoes. Oxidation of SO₂ in the atmosphere produces secondary sulfate aerosols, a major compound responsible for acid deposition and smog and haze. By scattering solar radiation and acting as cloud condensation nuclei, sulfate aerosols also directly and indirectly alter the radiation budget of the Earth.

Satellite retrievals of SO₂ began with Nimbus-7 Total Ozone Mapping Spectrometer (TOMS, Kruger, 1983). With measurements only at six discrete wavelengths, the TOMS SO₂ data record is generally limited to large volcanic eruptions. Starting from the 1990s, hyperspectral UV measurements made by instruments such as GOME (Global Ozone Monitoring Experiment) allow SO₂ absorption features to be more clearly separated from interfering processes, enabling the detection of anthropogenic SO₂ signal from space (e.g., Eisinger and Burrows, 1998). Since 2004, Dutch-Finnish Ozone Monitoring Instrument (OMI) onboard NASA's polar orbiting Aura satellite has been providing global monitoring of both anthropogenic and volcanic SO₂ with increased spatial resolution. The previous NASA standard OMI SO₂ product is based on discrete wavelength Band Residual Difference (BRD, Krotkov et al., 2006) and Linear Fit

(LF, Yang et al., 2007) algorithms. The new generation standard OMI SO₂ product (released in 2014 for anthropogenic SO₂ and in 2016 for volcanic SO₂) is based on the Principal Component Analysis (PCA) algorithm (Li et al., 2013; 2017) that offers significantly improved data quality. NMSO₂-PCA-L2 is based on the same PCA retrieval algorithm that has been implemented for Aura/OMI.

2. PRINCIPAL COMPONENT ANALYSIS SO₂ ALGORITHM

2.1 General Description

This section describes the Principal Component Analysis (PCA) SO₂ algorithm and its implementation with SNPP/OMPS. The algorithm has been described in detail elsewhere (Li et al., 2013; 2017) and is only briefly summarized here. In this algorithm, we apply a PCA technique to satellite measured backscattered UV (BUV) radiances between ~310 and 340 nm to derive spectral features from the measured spectra. These features, in the form of Principal Components (PCs), are related to various geophysical processes (e.g., ozone absorption, rotational Raman scattering) and instrument measurement details (e.g., wavelength shift, dark current). We use these PCs in SO₂ spectral fitting to reduce their interferences. It should be noted that BUV instruments such as OMI and OMPS have different sensitivities to SO₂ at different altitudes. In the absence of such information on the SO₂ plume height, for each OMPS pixel, the NMSO₂-PCA-L2 provides five estimates of the total SO₂ Vertical Column Density (VCD) in Dobson Units ($1 \text{ DU} = 2.69 \cdot 10^{16} \text{ molecules/cm}^2$), with each corresponding to a different assumed SO₂ cloud height or Center of Mass Altitude (CMA). All five VCD values represent the estimated total SO₂ burden within the entire atmospheric column. Therefore they should not be interpreted as partial column amounts within different layers or parts of the atmosphere. The five estimates are provided

so that data users may select the one or interpolate between the two estimates that are most representative of the conditions for a particular case of interest.

2.2 PBL SO₂ Retrieval

The Planetary Boundary Layer (PBL) SO₂ in NMSO₂-PCA-L2 is an estimated SO₂ VCD assuming that SO₂ is predominantly in the PBL or the lowest one km of the atmosphere. It is recommended for use in studies on near-surface pollution. For each OMPS orbit, we process its 36 rows (cross-track positions) one at a time, employing a PCA technique to extract Principal Components (PCs or v_i) for the spectral range 310.5-340 nm from the sun-normalized BUV radiance spectra. The PCs are ranked in descending order according to the spectral variance they each explain. If derived from SO₂-free regions, the first several PCs that account for the most of the variance are representative of geophysical processes unrelated to SO₂ such as ozone (O₃) absorption, as well as measurement details such as wavelength shift. We then obtain an estimate of SO₂ VCD (Ω_{SO_2}) and the coefficients of the PCs (ω) by fitting the first n_v (up to 15 non-SO₂) PCs and the SO₂ Jacobians ($\partial N / \partial \Omega_{SO_2}$) to the measured radiance spectrum (in this case the quantity N , which is the scaled logarithm of the sun-normalized radiances, I):

$$N(\omega, \Omega_{SO_2}) = \sum_{i=1}^{n_v} \omega_i v_i + \Omega_{SO_2} \frac{\partial N}{\partial \Omega_{SO_2}} \quad (1)$$

The SO₂ Jacobians represent the sensitivity of sun-normalized BUV radiances (I or its logarithm, N) at the Top Of Atmosphere (TOA) to a unit perturbation in Ω_{SO_2} , and were pre-calculated with a radiative transfer code. For the current NMSO₂-PCA-L2 PBL SO₂ VCD data, we use a fixed SO₂ Jacobian spectrum in Eq. (1), calculated assuming that SO₂ is predominantly in the lowest 1 km of the atmosphere and that the observation is made under cloud-free conditions with fixed surface albedo (0.05), surface pressure (1013.25 hPa), solar zenith angle

(30°), viewing zenith angle (0°), and pre-set O₃ and temperature profiles (with O₃ VCD = 325 DU). This simplification may lead to biases under certain conditions and data filtering is recommended before analysis (see below).

2.3 Volcanic SO₂ Retrieval

To facilitate studies on volcanic SO₂, NMSO2-PCA-L2 provides SO₂ VCD estimates assuming SO₂ plume heights or CMAs of 3 (lower troposphere, TRL), 8 (middle troposphere, TRM), 13 (upper troposphere, TRU), and 18 (lower stratosphere, STL) km. The first two assumed CMAs are typical of volcano degassing and moderate eruptions, respectively, whereas the latter two represent violent volcanic eruptions. For volcanic SO₂ retrievals, we use PBL SO₂ (section 2.2) and the Simple Lambertian Equivalent Reflectivity (SLER or R) derived from TOA radiances for each pixel as input. The SO₂ Jacobians as a function of solar zenith angle (θ_0), viewing zenith angle (θ), and relative azimuth angle (ϕ) can be calculated with the following equation:

$$\frac{\partial I}{\partial \Omega_{SO_2}} = \frac{\partial I_0(\theta_0, \theta)}{\partial \Omega_{SO_2}} + \frac{\partial I_1(\theta_0, \theta)}{\partial \Omega_{SO_2}} \cos \phi + \frac{\partial I_2(\theta_0, \theta)}{\partial \Omega_{SO_2}} \cos 2\phi + \frac{R}{(1-RS_b)} \frac{\partial I_r(\theta_0, \theta)}{\partial \Omega_{SO_2}} + \frac{R^2 I_r(\theta_0, \theta)}{(1-RS_b)^2} \frac{\partial S_b}{\partial \Omega_{SO_2}} \quad (2)$$

Here I_0 , I_1 , and I_2 represent the atmospheric contribution to the radiances (I). RI_r represents the TOA radiance that is reflected once from the surface and transmitted through the atmosphere, and $(1 - RS_b)$ accounts for the effects of multiple reflections between the surface and the atmosphere, with S_b being the fraction of the Lambertian surface-reflected radiation that is scattered back to the surface by the atmosphere. In addition, SO₂ Jacobians also depend on the amount and vertical profile of SO₂ and O₃.

In the retrieval algorithm, the SO₂ Jacobians are interpolated from a set of pre-calculated lookup tables for 21 climatology O₃ profiles and four presumed SO₂

profiles (i.e., TRL, TRM, TRU, and STL). The nodes of θ_0 (SZA), θ (VZA) and SO₂ in the lookup table are given in Table 1.

Table 1. Nodes of the Solar Zenith Angle (SZA), Viewing Zenith Angle (VZA), and SO₂ column amount, as used in the pre-computed SO₂ Jacobians lookup tables.

Parameter		Nodes													
SZA	0°	15°	30°	45°	60°	70°	77°	81°							
VZA	0°	15°	30°	45°	60°	70°	75°	80°							
SO ₂ (DU)	0	1	5	10	50	100	200	300	400	500	600	700	800	900	1000

For each OMPS pixel, the SO₂ Jacobians are first calculated from exact observational geometry, scene reflectivity, R , and PBL SO₂ for an initial estimate of the volcanic SO₂ VCDs. Next, the SO₂ VCD from the first step is used as an input to the lookup table to obtain updated estimates for SO₂ Jacobians and VCD. The iterations continue until the results converge (SO₂ VCD difference between two successive steps < 0.1 DU or 1% for pixels with SO₂ VCD > 100 DU) or the number of iterations exceeds the upper limit (15). The retrieval starts from a nominal fitting window of 313-340 nm. But for pixels with strong SO₂ signals (e.g., large eruptions), the fitting window is optimized for each iteration step to exclude shorter wavelengths that are saturated (i.e., SO₂ Jacobians become significantly smaller with increasing SO₂ VCD). This optimal fitting window helps to reduce the interpolation error in SO₂ Jacobians and also the low bias in LF retrievals. The same data processing steps are applied separately for the TRL, TRM, TRU, and STL SO₂ VCD estimates.

2.4 Data Quality Assessment and Data Filtering

Errors in NMSO2-PCA-L2 data can arise from both the input radiance data and the SO₂ Jacobians used in retrievals. We estimate the retrieval noise by

calculating the standard deviation over presumably SO₂-free remote regions (e.g., the equatorial Pacific). We have also conducted extensive comparison between NMSO₂-PCA-L2 and the OMI PCA SO₂ data, and found generally good agreement between the two products (Li et al., 2017; Zhang et al., 2017), despite large differences in instrument spectral and spatial resolution.

For data analysis, we recommend that all pixels with large solar zenith angle (SZA > 70) or near the edge of the swath (rows 1-2 and 35-36) or significantly affected by the South Atlantic Anomaly (flag_SAA = 1) be excluded. There are also occasional stripes (unphysical, large positive or negative values for a large portion of a row) due to retrieval artifacts, and those affected pixels should be excluded in data analysis.

ColumnAmountSO2_PBL: As a measurement of retrieval noise, the pixel-level standard deviation is ~0.2-0.3 DU over the presumably SO₂-free equatorial Pacific for PBL SO₂. For PBL SO₂, because of the simplification in Jacobians mentioned above, we also recommend that only snow/ice free pixels with relatively small RadiativeCloudFraction (< 0.3) be used.

ColumnAmountSO2_TRL: Due to increased sensitivity to elevated SO₂, the pixel-level standard deviation in TRL data is estimated at ~0.1 DU under optimal observational conditions in the tropics. The noise is about 0.15 DU for high latitudes. The data can be used for cloudy, clear and mixed scenes as well as for elevated terrain, but will overestimate SO₂ amounts if SO₂ cloud altitude is higher than 3 km. The TRL data can be used for studies of volcanic degassing.

ColumnAmountSO2_TRM: The standard deviation of TRM retrievals in background areas is generally < 0.1 DU. Like the TRL data, the TRM data can be used for various sky conditions. The TRM data can be used for investigating SO₂ plumes from moderate eruptions, but will overestimate SO₂ amounts if SO₂ cloud altitude is higher than ~8 km.

ColumnAmountSO2_TRU data are intended for use for explosive volcanic eruptions where SO₂ is injected into the upper troposphere. The standard deviation over background areas is < 0.1 DU for all latitudes for TRU data. The TRU data can be used for investigating SO₂ clouds from explosive eruptions in upper troposphere and tropopause in mid- and high latitudes, but will overestimate SO₂ amounts if SO₂ cloud CMA is higher than ~13 km.

ColumnAmountSO2_STL data are intended for use for explosive volcanic eruptions where SO₂ is injected directly into the lower stratosphere at 16-20km. STL data will underestimate total SO₂ amounts for lower SO₂ cloud altitudes. The standard deviation over background areas is < 0.1 DU for all latitudes for STL data.

2.5 Updates in Version 1.2

A key requirement in the PCA-based SO₂ retrieval approach is that the PCs derived from the radiance data and subsequently used in spectral fitting represent only non SO₂ features. Since globally SO₂ signals are relatively weak over most areas most of the time, this requirement is met in the vast majority of situations. One rare but notable exception occurs when volcanic eruptions emit large amounts of SO₂ into the atmosphere. Strong absorption of UV radiation by SO₂ from these eruptions cause significant changes in the Earthshine radiances measured by the OMPS instrument. As a result, PCs derived from those radiance data often contain strong SO₂ related spectral features.

In version 1.1 NMSO2-PCA-L2 product, we implemented a scheme to exclude these SO₂-contaminated PCs in spectral fitting by examining the correlation between the PCs and SO₂ cross sections. While this check is effective for a number of volcanic eruptions observed by OMPS during 2012-2019, we also note that

retrievals for some particularly large eruptions can still be problematic (see Figure 1a for an example).

In version 1.2, we have added a new volcanic SO₂ flagging scheme to detect OMPS pixels with substantial volcanic SO₂ signals. This scheme is based on the differences in ozone retrieval residuals from two wavelength pairs (313 and 314 nm, and 314 and 315 nm). The residuals represent the differences between the measured and calculated radiances at different wavelengths in an ozone retrieval that assumes little or no SO₂ in the atmosphere. Under most conditions, this is a valid assumption and the residuals are similar between, for example, 313 and 314 nm. In the presence of large amounts of SO₂ from volcanic eruptions, however, the residuals are much greater at 313 nm than at 314 nm, as SO₂ absorbs much more strongly at the former wavelength. Tests with OMPS data have shown that the scheme can effectively detect pixels with ~5 DU of SO₂ in the stratosphere.

In version 1.2 NMSO2-PCA-L2 product, this new volcanic SO₂ flagging scheme is run first and the OMPS pixels flagged by the scheme are excluded from the PCA analysis. This helps to minimize the impacts of large volcanic eruptions and significantly improves retrievals in those situations (see Figure 1b).

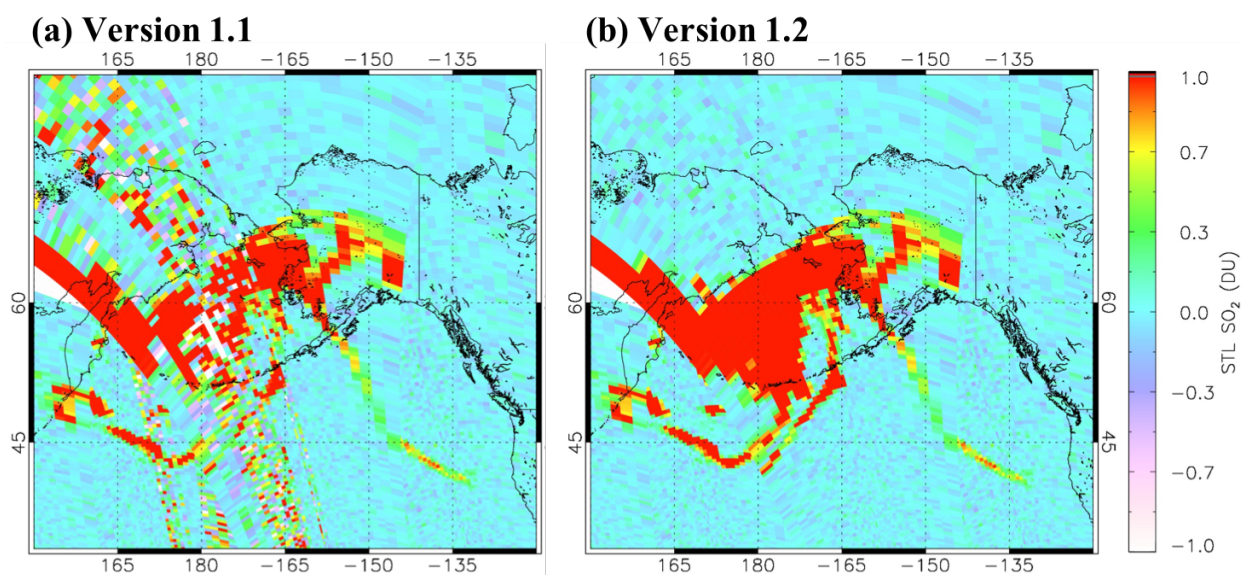


Figure 1. The volcanic SO₂ flagging scheme implemented in NMSO2-PCA-L2 version 1.2 significantly improves retrieval quality for some large eruptions. The example in the figure shows STL (18-km *a priori* profile) SO₂ retrievals for the Raikoke plume on June 24, 2019 in (a) version 1.1 and (b) version 1.2 of the NMSO2-PCA-L2 product.

3. DATASET ORGANIZATION

The NMSO2-PCA-L2 product is a set of Level 2 orbital swath files that follow a specific file naming convention and dataset organization.

3.1 File Naming Convention

The NMSO2-PCA-L2 product files are named as in this example:

OMPS-NPP_NMSO2-PCA-L2_v1.0_2017m0601t171237_o29118_2017m1013t150510.h5

The components of the filename are as follows:

1. Instrument (OMPS)
2. Spacecraft (NPP)
3. Product Name (NMSO2-PCA-L2)
4. Product Version (1.0)
5. Date and Time at Start of Orbit (2017-06-01 17:12:37 UTC)
6. Orbit Number (29118)
7. Production Date and Time (2017-10-13 15:05:10 UTC)
8. File Type (h5)

3.2 File Format and Structure

The NMSO2-PCA-L2 product files are in plain HDF5 that is netCDF4-compatible and CF-compliant. Each product file contains global attributes,

dimensions, an ancillary data group, a geolocation data group, and a science data group.

3.3 Key Science Datasets

There are five key science datasets in the science data group in each NMSO2-PCA-L2 product file that correspond to the five estimates of the total vertical column amount (VCD) of SO₂ assuming specific cloud height.

3.3.1 *ColumnAmountSO2_PBL*

ColumnAmountSO2_PBL is the estimated total VCD of SO₂ in DU assuming that the observed SO₂ lies within the lowest kilometer of the atmosphere.

3.3.2 *ColumnAmountSO2_TRL*

ColumnAmountSO2_TRL is the estimated total VCD of SO₂ in DU assuming a center of mass altitude of 3 km.

3.3.3 *ColumnAmountSO2_TRM*

ColumnAmountSO2_TRM is the estimated total VCD of SO₂ in DU assuming a center of mass altitude of 8 km.

3.3.4 *ColumnAmountSO2_TRU*

ColumnAmountSO2_TRU is the estimated total VCD of SO₂ in DU assuming a center of mass altitude of 13 km.

3.3.5 *ColumnAmountSO2_STL*

ColumnAmountSO2_STL is the estimated total VCD of SO₂ in DU assuming a center of mass altitude of 18 km.

4. DATA CONTENTS

Each NMSO2-PCA-L2 product file contains global attributes, dimensions, an ancillary data group, a geolocation data group, and a science data group.

4.1 Global Attributes

There are 42 global attributes in each NMSO2-PCA-L2 product file as shown in Figure 2.

Number of attributes = 42		Add	Delete
Name	Value	Type	Array Size
AuthorAffiliation	NASA/GSFC	String, length = 9	Scalar
AuthorName	N. Krotkov, et al.	String, length = 18	Scalar
Conventions	CF-1.6	String, length = 6	Scalar
DataSetQuality	Under investigation.	String, length = 20	Scalar
DayNightFlag	Day	String, length = 3	Scalar
EastBoundingCoordinate	180.0	32-bit floating-point	1
EquatorCrossingDate	2017-06-10	String, length = 10	Scalar
EquatorCrossingLongitude	-61.39519	32-bit floating-point	1
EquatorCrossingTime	17:30:41.606	String, length = 12	Scalar
FOVResolution	50x50km	String, length = 7	Scalar
GranuleDay	10	32-bit integer	1
GranuleDayOfYear	161	32-bit integer	1
GranuleMonth	6	32-bit integer	1
GranuleYear	2017	32-bit integer	1
HDFVersion	5-1.8.17	String, length = 8	Scalar
InputPointer	OMPS-NPP_NMEV-L1B-p000_v2.0_2017m0610t171237_o29118_2017m0610t203523....	String, length = 139	Scalar
InstrumentShortName	OMPS	String, length = 4	Scalar
LocalGranuleID	OMPS-NPP_NMSO2-PCA-L2_v1.0_2017m0610t171237_o29118_2017m1013t150510.h5	String, length = 70	Scalar
LocalityValue	Global	String, length = 6	Scalar
LongName	OMPS/NPP PCA SO2 Total Column 1-Orbit L2 Swath 50x50km	String, length = 54	Scalar
NorthBoundingCoordinate	89.650276	32-bit floating-point	1
NumberOfTimes	320	32-bit integer	1
OrbitNumber	29118	32-bit integer	1
PGEVersion	0.0.9	String, length = 5	Scalar
ParameterName	Vertical Column Sulfur Dioxide	String, length = 30	Scalar
PlatformShortName	Suomi-NPP	String, length = 9	Scalar
ProcessLevel	2	String, length = 1	Scalar
ProcessingCenter	ACPS	String, length = 4	Scalar
ProductType	L2 Swath	String, length = 8	Scalar
ProductionDateTime	2017-10-13T15:05:10.0Z	String, length = 22	Scalar
RangeBeginningDate	2017-06-10	String, length = 10	Scalar
RangeBeginningTime	17:24:17.876	String, length = 12	Scalar
RangeEndingDate	2017-06-10	String, length = 10	Scalar
RangeEndingTime	18:04:06.638	String, length = 12	Scalar
SensorShortName	Nadir Mapper	String, length = 12	Scalar
ShortName	OMPS_NPP_NMSO2_PCA_L2	String, length = 21	Scalar
Source	Suomi-NPP OMPS Nadir Mapper	String, length = 27	Scalar
SouthBoundingCoordinate	-26.10196	32-bit floating-point	1
VersionID	1	String, length = 1	Scalar
WestBoundingCoordinate	-180.0	32-bit floating-point	1
identifier_product_doi	10.5067/MEASURES/SO2/DATA203	String, length = 28	Scalar
identifier_product_doi_authority	http://dx.doi.org/	String, length = 18	Scalar

Figure 2. Global Attributes

4.2 Dimensions

There are four dimensions in each NMSO2-PCA-L2 product file:

- nTimes - The dimension representing the along-track-line number.
- nWavel2 - The dimension representing the wavelengths for the fitting windows.
- nWavel3 - The dimension representing the wavelengths for SLER and dN/dR.
- nXtrack - The dimension representing the cross-track-position number.

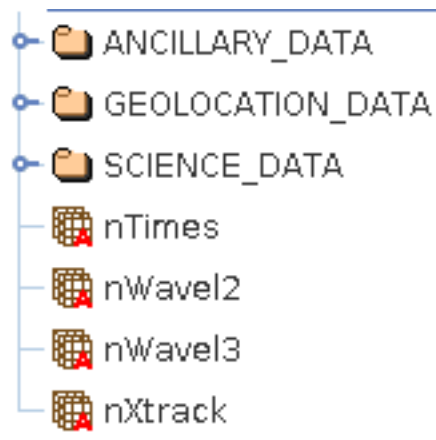


Figure 3. Groups and Dimensions

4.3 Data Fields

4.3.1 Ancillary Data

There are two datasets, CloudPressure and TerrainPressure, in the ancillary data group in each NMSO2-PCA-L2 product file as shown in Figure 4.

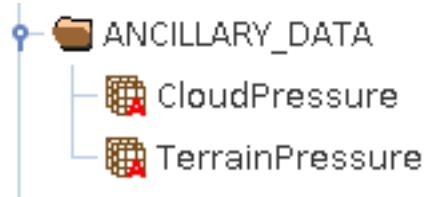


Figure 4. Ancillary Data Group

4.3.2 Geolocation Data

There are eleven datasets in the geolocation data group in each NMSO2-PCA-L2 product file as shown in Figure 5.

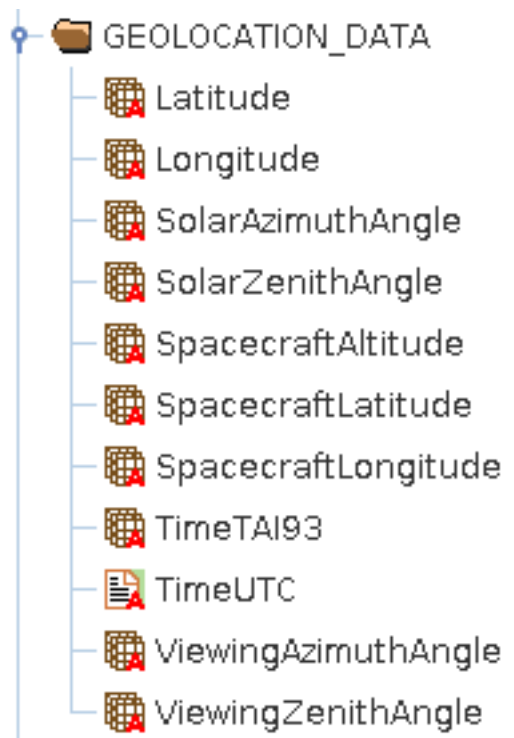


Figure 5. Geolocation Data Group

4.3.3 *Science Data*

There are 20 datasets in the science data group in each NMSO2-PCA-L2 product file as shown in Figure 6.

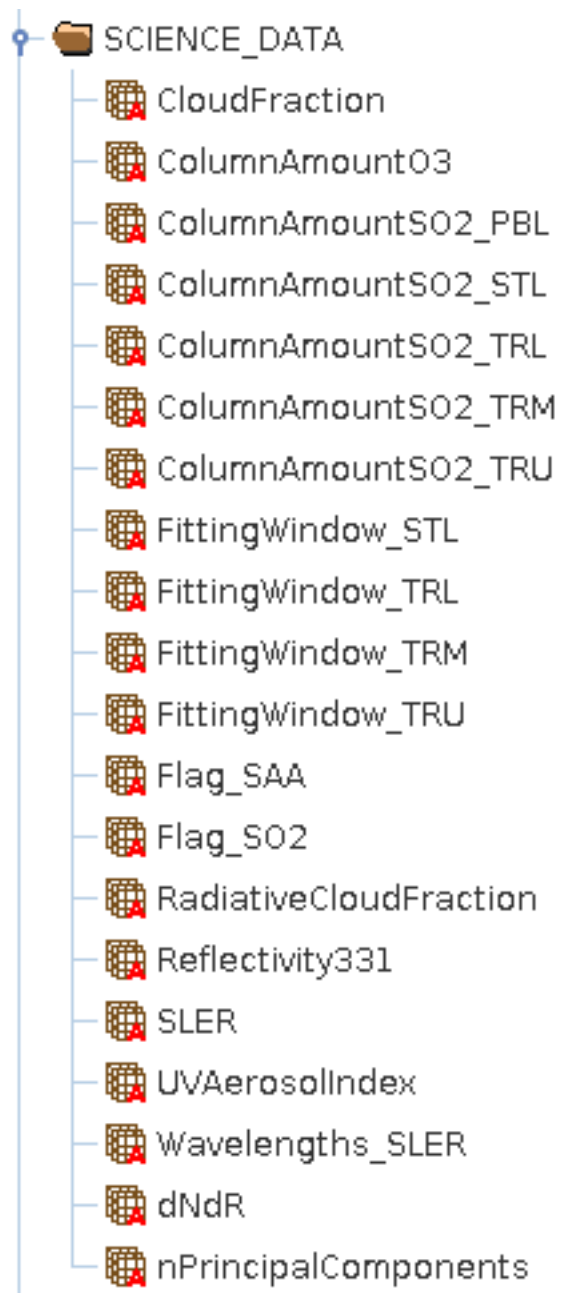


Figure 6. Science Data Group

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